

1 Application: xia2setup

1.1 Introduction

xia2setup is a new application which will “trawl” a directory and construct a .xinfo file to reduce the data that is found, with the following assumptions:

- All data in a directory is measured from one crystal.
- The date and time of data collection is in the image header.
- If a sequence (.seq) file is found in the directory this corresponds to the sequence of that crystal.
- If a scan (.scan) file is found this corresponds to the wavelengths of the data which were collected.
- Heavy atom information will be passed in on the command line.

This will give a command line something like:

```
xia2setup -atom se -beam x,y -project foo -crystal bar /path/to/directory
```

This will generate a .xinfo file called automatic.xinfo which should be inspected and perhaps updated before being used. If heavy atom information and a scan are supplied then the system will try to identify PEAK, INFLECTION, LOW and HIGH REMOTE data sets, or SAD if appropriate, else for single wavelength sets this will be called “NATIVE” or WAVE1 ...

Sweeps are named SWEEP1 ... SWEEP N , since the names of sweeps are not recorded beyond the integration stage.

1.2 Identification of Wavelengths

If an edge scan is supplied then CHOOCH is run to identify the f' and f'' values as well as the peak and inflection point. Wavelengths are scanned, and the nearest to the inflection and peak is identified as such, with a 0.001Å margin. Beyond this range, the wavelength is identified as a low or high remote - in which case the form factors will be identified by CROSSEC.

This now basically works, though more work is needed to make it less horrible.

1.3 Additional Functionality

It would be nice if the following functions could be added to this program:

- Determination of beam centre with labelit.screen.

- Determination of MASK parameters with diffraction image viewer.

This would allow improvement in the actual data reduction and a more intuitive interface for the user.